

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 3.72

Global applicability domain: Inside

Local applicability domain index: 4.24e-01

Confidence level: 7.12e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Dalapon-sodium</div> <div>Measured: 7.24</div> <div>Predicted: 5.61</div>	<div>Image not found</div> <div>2-Chlorobenzoic acid</div> <div>Measured: 10.0</div> <div>Predicted: 3.89</div>	<div>Image not found</div> <div>Trichloroacetic acid</div> <div>Measured: 1.70</div> <div>Predicted: 2.22</div>
<div>Image not found</div> <div>2,6-Dichlorobenzoic acid</div> <div>Measured: 1.82</div> <div>Predicted: 3.59</div>	<div>Image not found</div> <div>3,4-Dichlorobenzoic acid</div> <div>Measured: 2.29</div> <div>Predicted: 3.54</div>	